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Attorney Docket No.: 9476-003-999

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Sir:

Prior to prosecution on the merits, please amend the specification and pending claim and insert new claims as indicated. This amendment is accompanied by (a) Appendix A showing amended paragraphs of the specification; (b) Appendix B showing amendments to Claim 1; (c) Appendix C showing all currently pending claims after entry of this amendment; (d) an Information Disclosure Statement; (e) PTO form 1449 and copies of cited references AA–BY; and (f) fee transmittal sheet.

In The Specification

Please amend the specification as follows:

Replace the paragraph beginning at page 8, line 5 with:

An additional aspect considered by Mestres et al. is the issue of molecules existing in multiple structural conformations, i.e. energetically there may be more than one possible structure for a given molecule. Mestres et al. calculate the similarity indexes of all pairs of conformations